Propanedioic acid, bromomethyl-, diethyl ester

Other names: Diethyl bromomethylmalonate
Diethyl 2-bromo-2-methylmalonate
Diethyl methylbromomalonate
Malonic acid, bromomethyl-, diethyl ester
propanedioic acid, 2-chloro-2-methyl-, diethyl ester

Inchi: InChI=1S/C8H13BrO4/c1-4-12-6(10)8(3,9)7(11)13-5-2/h4-5H2,1-3H3

InchiKey: CSLQAXTUGPUBCW-UHFFFAOYSA-N

Formula: C8H13BrO4

SMILES: CCOC(=O)C(C)(Br)C(=O)OCC

Mol. weight [g/mol]: 253.09

CAS: 29263-94-3

Physical Properties

Property code	Value	Unit	Source
gf	-434.20	kJ/mol	Joback Method
hf	-680.47	kJ/mol	Joback Method
hfus	19.92	kJ/mol	Joback Method
hvap	56.85	kJ/mol	Joback Method
log10ws	-1.44		Crippen Method
logp	1.266		Crippen Method
mcvol	155.960	ml/mol	McGowan Method
pc	3065.95	kPa	Joback Method
tb	597.95	K	Joback Method
tc	805.44	K	Joback Method
tf	386.46	K	Joback Method
vc	0.583	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	362.82	J/mol×K	597.95	Joback Method
cpg	374.23	J/mol×K	632.53	Joback Method
cpg	384.98	J/mol×K	667.11	Joback Method
cpg	395.08	J/mol×K	701.70	Joback Method

cpg	404.55	J/mol×K	736.28	Joback Method
cpg	413.41	J/mol×K	770.86	Joback Method
cpg	421.66	J/mol×K	805.44	Joback Method
dvisc	0.0016474	Pa×s	386.46	Joback Method
dvisc	0.0009962	Pa×s	421.71	Joback Method
dvisc	0.0006511	Pa×s	456.96	Joback Method
dvisc	0.0004522	Pa×s	492.21	Joback Method
dvisc	0.0003298	Pa×s	527.45	Joback Method
dvisc	0.0002502	Pa×s	562.70	Joback Method
dvisc	0.0001961	Pa×s	597.95	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C29263943&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume